



U.S. DEPARTMENT OF
ENERGY

The View from Germantown



**Betsy A. Riley, DOE-ASCR
Program Manager for ALCF**

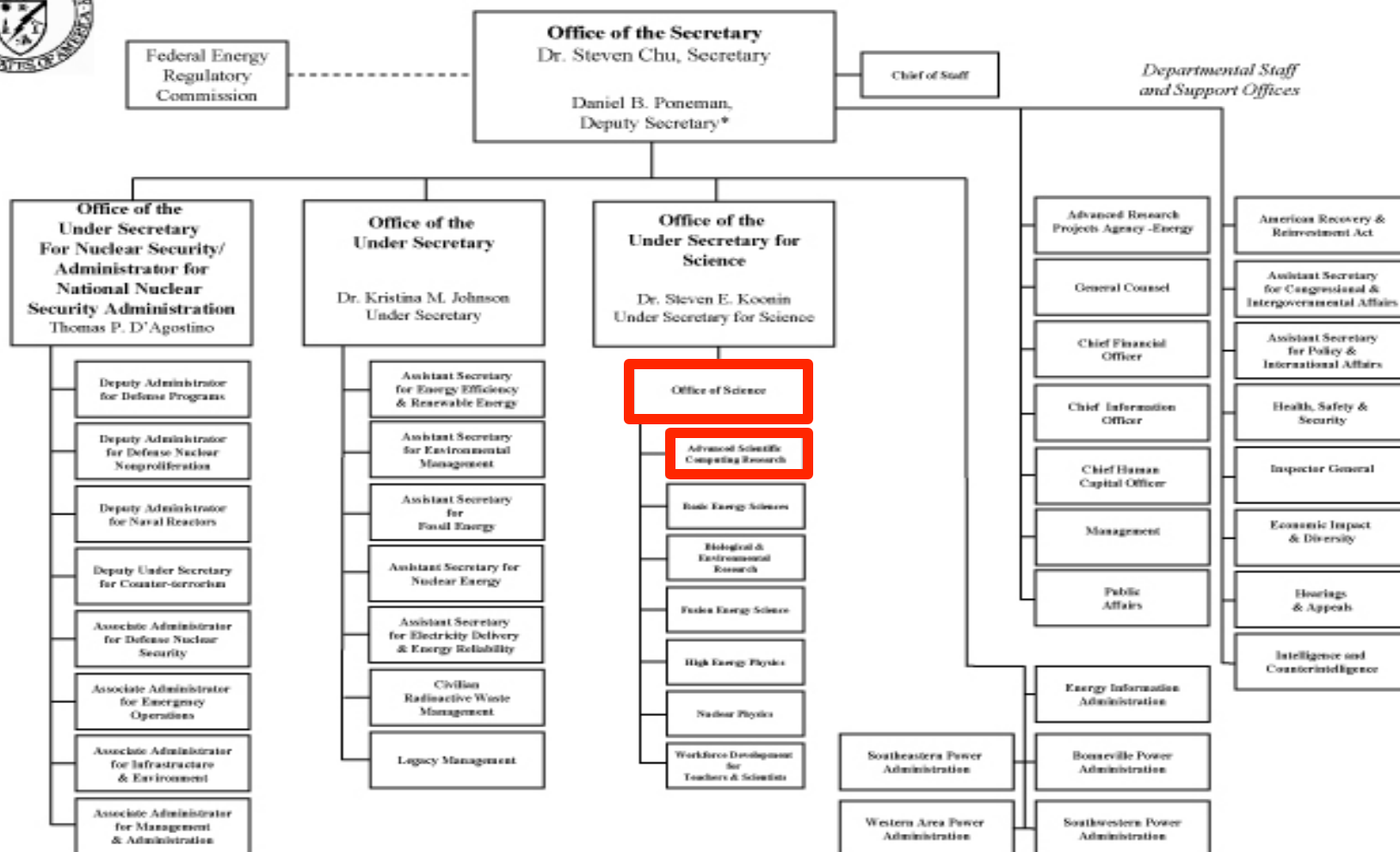
Getting Started Workshop -- January 18, 2011



DOE Organization Chart



DEPARTMENT OF ENERGY



* The Deputy Secretary also serves as the Chief Operating Officer



INCITE Background

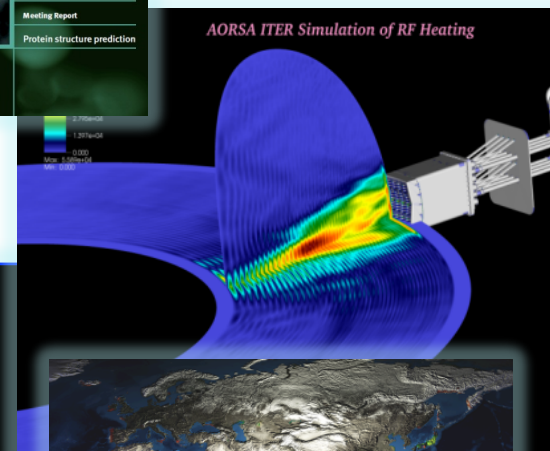
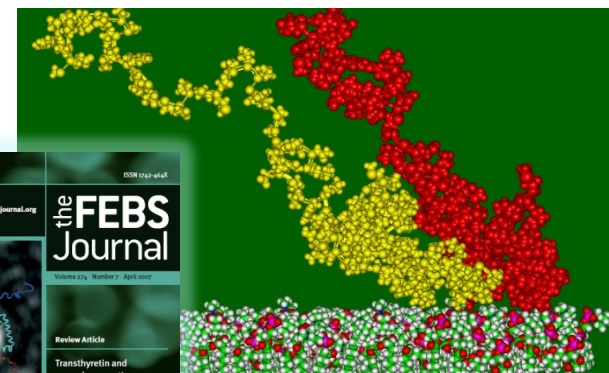
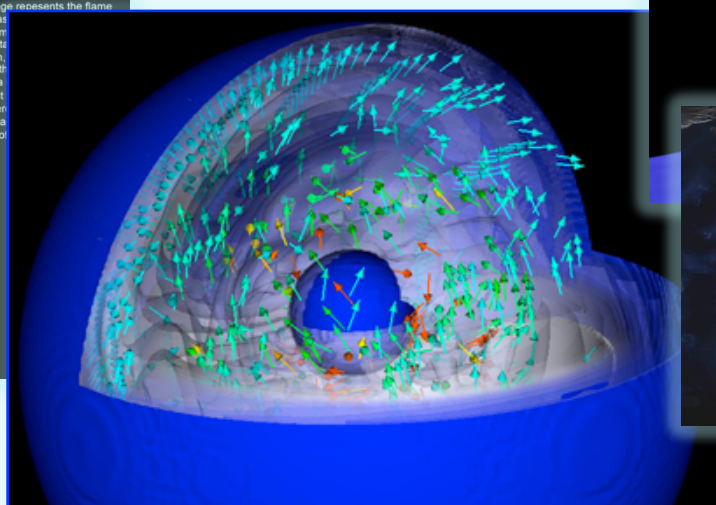
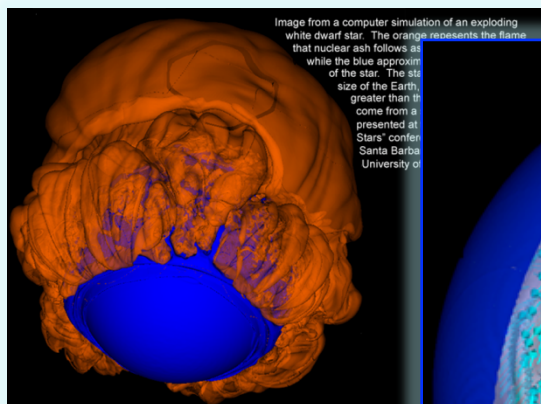
- Began in 2004 at LBNL's National Energy Scientific Computing Center (NERSC) – now used for Argonne (ALCF) and Oak Ridge (OLCF) allocations.
- Provides Office of Science computing resources to a small number of **computationally intensive** research projects of **large scale**, that can make **high-impact scientific advances** through the use of a large allocation of computer time and data storage
- Open to U.S. and international researchers, including industry
- Does not require (or provide) DOE Office of Science funding
- Selected by peer and computational reviews



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Your projects have been chosen

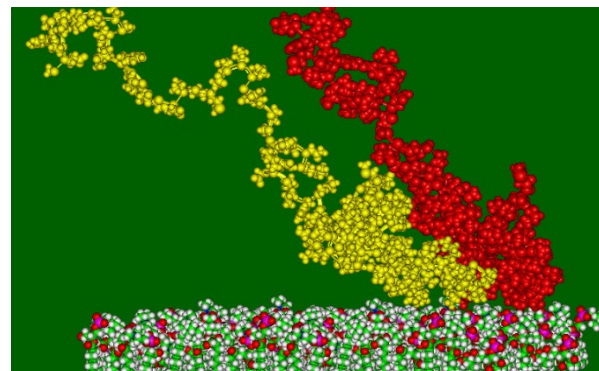
ASCR allocates facility
resources through INCITE
so that researchers can
DO SCIENCE
in important areas



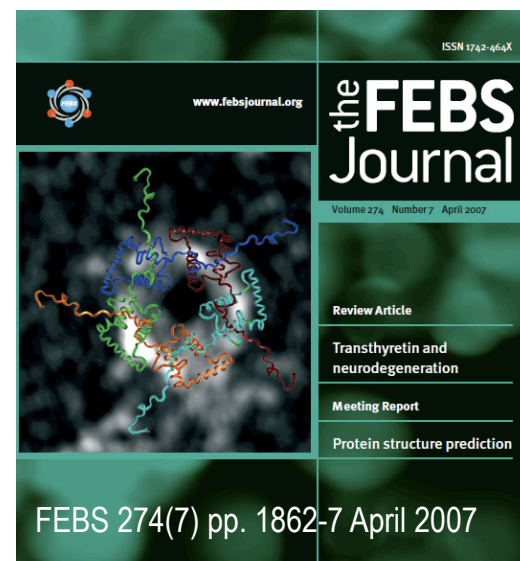


Modeling of Protofibril Structures Provides Insight into Molecular Basis of Parkinson's Disease

- PI: Igor Tsigelny, UCSD
- Parkinson's Disease is the 2nd most common adult neurological disease
- Increased aggregation of *alpha-synuclein* protein is thought to lead to harmful pore-like structures in human membranes
- UCSD - SDSC team used molecular modeling and molecular dynamics simulations in combination with biochemical and ultrastructural analysis to show that *alpha-synuclein* can lead to the formation of pore-like structures on membranes
- Used NAMD and MAPAS on Blue Gene/L at ALCF and SDSC



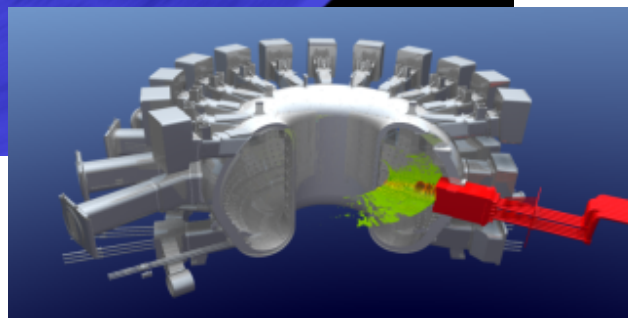
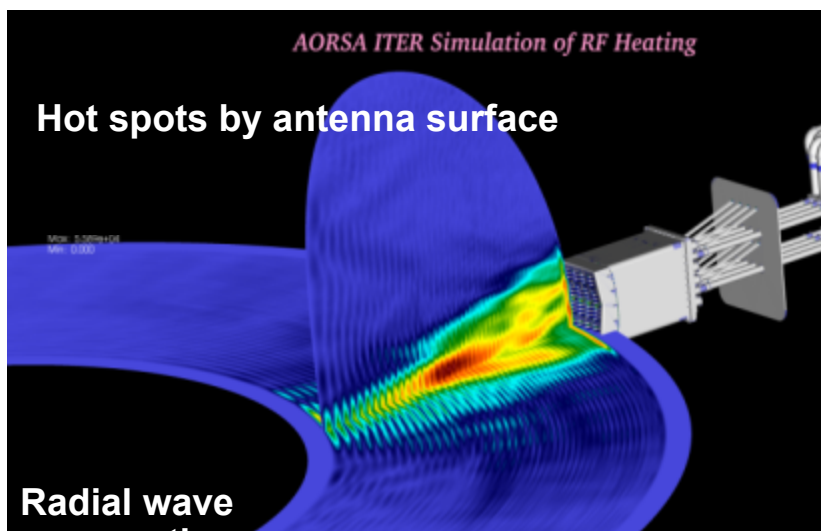
Above - formation of alpha-synuclein dimer on a membrane, aggregating toward the pentamer pore structure - below.





Producing New Insights for RF Heating of ITER Plasmas

“Until recently, we were limited to two-dimensional simulations. The larger computer [Jaguar] has allowed us to achieve three-dimensional images and validate the code with observations.” – Fred Jaeger, ORNL



- 3D simulations reveal new insights
 - “Hot spots” near antenna surface
 - “Parasitic” draining of heat to the plasma surface in smaller reactors
- Work pushing the boundaries of the system (22,500 processor cores, 87.5 TF) and demonstrating
 - Radial wave propagation and rapid absorption
 - Efficient plasma heating
- AORSA’s predictive capability can be coupled with Jaguar power to enhance fusion reactor design and operation for an unlimited clean energy source

Fully 3-dimensional simulations of plasma shed new light on the behavior of superheated ionic gas in the multibillion-dollar ITER fusion reactor

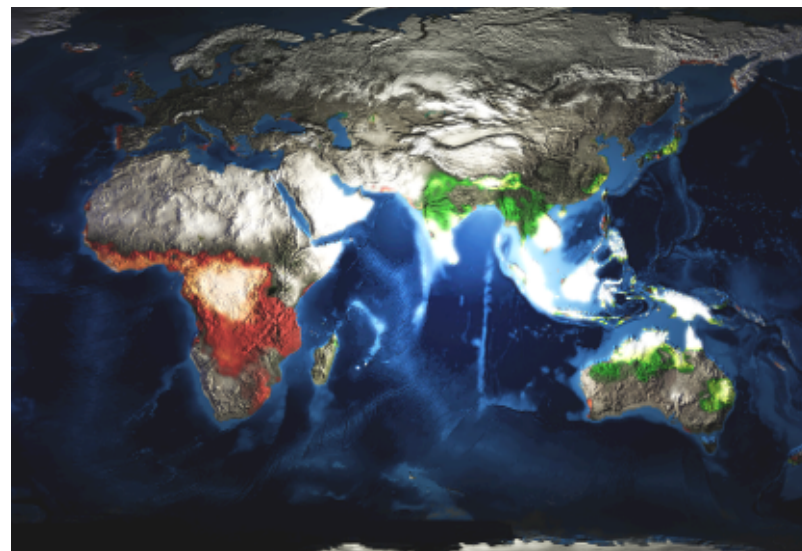


- **PI– Warren Washington, NCAR**
- **First-ever control runs of CCSM 3.5 at groundbreaking speed**

“[On Jaguar,] we got 100-year runs in three days. This was a significant upgrade of how we do science with this model. 40 years per day was out of our dreams.”

Peter Gent of NCAR, Chairman of CCSM Scientific Steering Committee, during keynote at CCSM Workshop, June 19, 2007

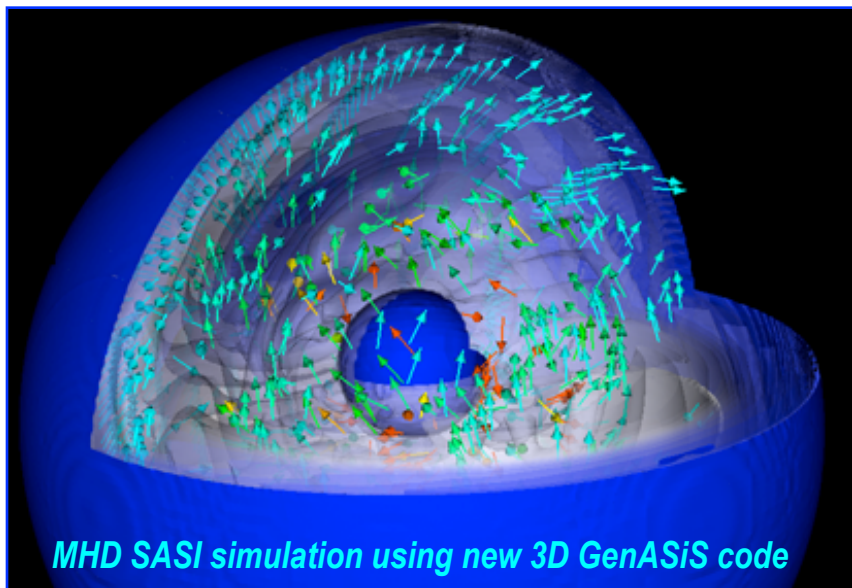
- **Major improvements in CCSM 3.5**
 - Arctic and Antarctic sea ice: Will the Arctic be ice free in summer of 2050?
 - Surface hydrology of land, critical for predictions of drought
- **Positioned to test full carbon-nitrogen cycle**



Instantaneous net ecosystem exchange (NEE): eastern half is in sunlight and the terrestrial ecosystems are taking up carbon (negative NEE, shown in green to bright white). Meanwhile, the sun has not yet risen in the western half of the image where the ecosystems are only respiring (positive NEE, shown in red)



Discovering the Elusive Core Collapse Supernova Explosion Mechanism



Researchers can now simulate ~1 second after 'post-bounce'. Petascale systems will allow longer simulations: tens of seconds after the explosion and will allow inclusion of neglected yet important physics such as magnetic fields.

- PI: Tony Mezzacappa, ORNL
- Achieved longer run simulations and, 0.8 seconds after explosion, saw the initial shock wave revived by turbulence of in-falling material
- CHIMERA used to investigate multiple stellar models, effect of both Newtonian and Einsteinian gravity, and impact of recently discovered subatomic physics
 - >12K cores used in current 3D simulations
- Current 3D spatial resolution
 - 78x156x312 (Chimera)
 - 256x256x256 (Genasis)

Researchers glean unprecedented insight into the shock waves that blow apart a 10- to 20-solar mass star



- **PI: Don Lamb, University of Chicago's Center for Astrophysical Thermonuclear Flashes**
- **First 3-dimensional detonation of white dwarf confirming that stars detonate in a supersonic process resembling diesel-engine combustion.**

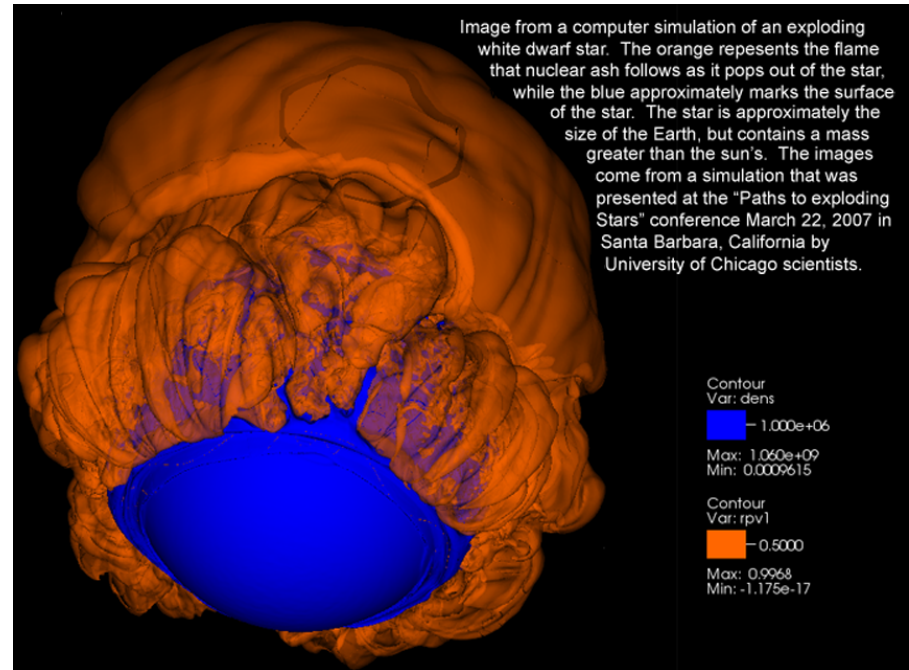


Image courtesy of Cal Jordan/University of Chicago Flash Team

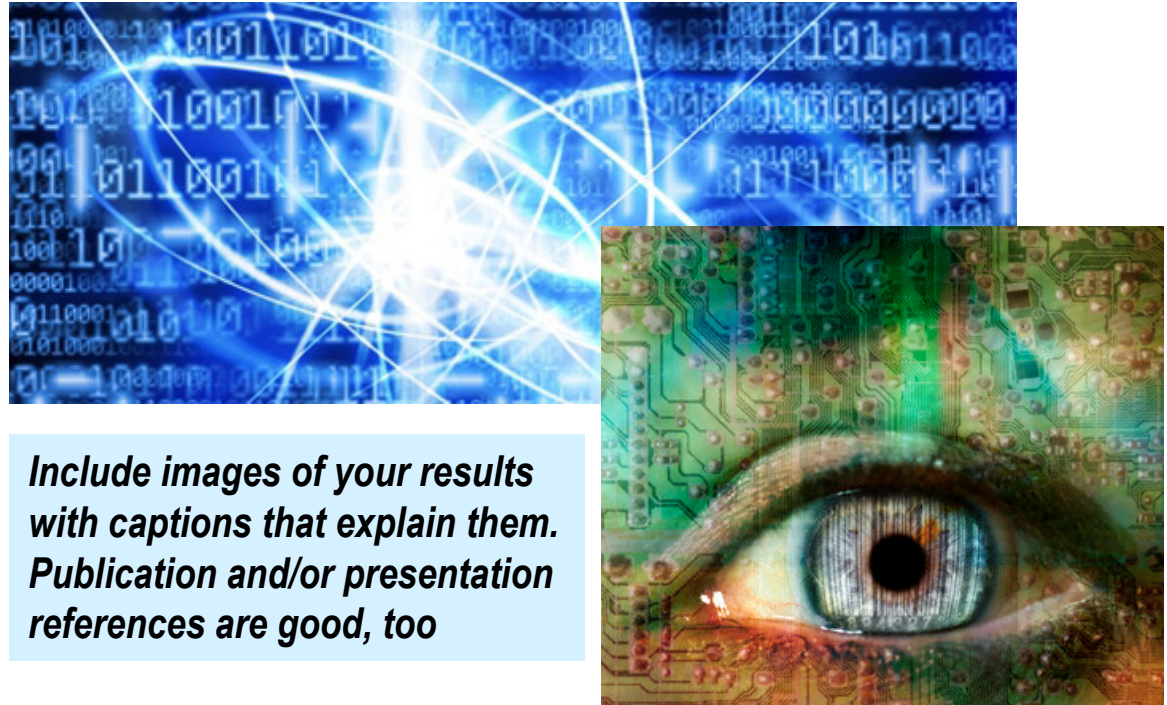
"We could not have asked for better or more support than we got from the folks at NERSC, in helping us to get on the NERSC machines quickly, in giving the job special status, and in helping us meet the challenges of running a large job on Bassi."

Don Lamb, University of Chicago's Center for Astrophysical Thermonuclear Flashes



Show us your Science!

- PI name & Organization
- What you achieved
(be specific, quantify)
- Why we care
(why it is important)
- How ALCF helped
(scaling? porting?)
- Resources used
(nodes, bytes, flops)



*Include images of your results
with captions that explain them.
Publication and/or presentation
references are good, too*



***“Honk your
own horn!”***